

1-Nitrobutane

627-05-4 | DTXSID8020967

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 7.93e-01

Global applicability domain: Inside

Local applicability domain index: 6.27e-01

Confidence level: 8.77e-01

Nearest Neighbors from the Training Set

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2-Butanone oxime

Measured: 0.7

Predicted: 7.27e-01

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2-Nitropropane

Measured: 0.92

Predicted: 8.70e-01

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Furan

Measured: 0.7

Predicted: 6.89e-01

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Thiophene

Measured: 0.95

Predicted: 8.25e-01

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Diethyl ether

Measured: 0.73

Predicted: 6.74e-01